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Nature of size-dependent lattice distortions in doped CeO2

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Abstract

Electron paramagnetic resonance spectroscopy of Gd3+ probe ions is used to investigate the nature of size dependent lattice distortions in bulk and nanocrystalline CeO2 with crystallite sizes of 600 and 10 nm, respectively, and doped with 0.5 and 1 cation% Y. The Gd3+ ions in bulk CeO2 are primarily located in almost perfect cubic crystal field, and the presence of the nearest neighbor vacancies results in trigonal distortion of this crystal field. In contrast, for nanocrystalline ceria, although the long-range symmetry remains unchanged, decreasing size results in local distortion of the crystal-field that is significantly different than that induced by the presence of nearest-neighbor oxygen vacancies. Different types of distortions are observed for the cation sites in the core and the surface regions of the nanocrystallites. Such lattice distortions at short-range are fundamental to the nanocrystalline state, being related to the increased ratio of the surface:bulk energy at nanometer length scales and provides mechanistic understanding of previously reported lattice parameter changes and phase transitions in nanocrystalline oxides.

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